

Supplementary Table 1

	NMRDraw Peak Detection Levels (Intensity)	Minimum Detected Volume	Median Detected Volume	Maximum Detected Volume
Lowest Contour Level				
CBCACONH	3.12E+06	7.E+05	6.E+07	2.E+09
HNCACB	1.01E+06	1.E+06	5.E+06	2.E+08
HNCACO	2.21E+06	2.E+06	1.E+07	4.E+08
HNCO*	5.15E+06	5.E+06	5.E+07	5.E+08
Intermediate Contour Level (2* Lowest Contour Level)				
CBCACONH	6.24E+06	6.E+06	9.E+07	2.E+09
HNCACB	2.02E+06	2.E+06	8.E+06	2.E+08
HNCACO	4.42E+06	2.E+06	2.E+07	4.E+08
HNCO	1.03E+07	1.E+07	7.E+07	5.E+08
Highest Contour Level (4* Lowest Contour Level)				
CBCACONH	1.25E+07	1.E+07	1.E+08	2.E+09
HNCACB	4.04E+06	4.E+06	1.E+07	2.E+08
HNCACO	8.83E+06	9.E+06	5.E+07	4.E+08
HNCO	2.06E+07	2.E+07	8.E+07	5.E+08

* Note that the HNCO detection level at Lowest Contour Level was mistakenly set to 5.15E+06 rather than 5.015E+06. This (< 3%) difference is not expected to significantly impact the resulting observations.

All other NMRDraw parameters for peak-picking were set to the default values:

Detection: X(+/-1) Y(+/-1) Z(+/-1)
 Interpolation: X(+/-1) Y(+/-1) Z(+/-1)
 Position Tolerances: X(2.0) Y(2.0) Z(2.0)
 Sinc Detect ON, Height Adjustments: X(1.200) Y(1.800) Z(1.800)
 Sinc Detect Linewidths: X(15.0Hz) Y(5.0Hz) Z(0.0Hz)